EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	15627	HARRISON.in. GIERASCH.in. VERDINE.in. "SHI.in. "	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 15:55
L2	34	l1 and opioid	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:07
L3	1114	564/123 564/161 564/170 564/171 564/174	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:08
L4	0	l3 and l1	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:08
L5	0	l3 and l2	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:08
L6	18	l3 and opioid	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:08
L7	18	l6 not l2	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:12
L8	80	endomorphin-2	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:12
L9	1	l8 and l1	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:13

EAST Search History

L10	0	l8 and l3	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:13
L11	77	l8 and derivat$	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:13
L12	40	l8 and opioid	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:13
L13	37	l11 and opioid	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:14
L14	36	l13 not l2	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:14
L15	36	l14 not l6	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2006/11/10 16:14

STN

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptayvv1621

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS	4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS	5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS	6	SEP 11	CA/CAplus enhanced with more pre-1907 records
NEWS	7	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS	8	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS	9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS	10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS	11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS	12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS	13	OCT 19	E-mail format enhanced
NEWS	14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS	15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	18	NOV 03	JAPIO enhanced with IPC 8 features and functionality

NEWS EXPRESS	NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:54:55 ON 10 NOV 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:55:12 ON 10 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 NOV 2006 HIGHEST RN 912878-87-6
DICTIONARY FILE UPDATES: 9 NOV 2006 HIGHEST RN 912878-87-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

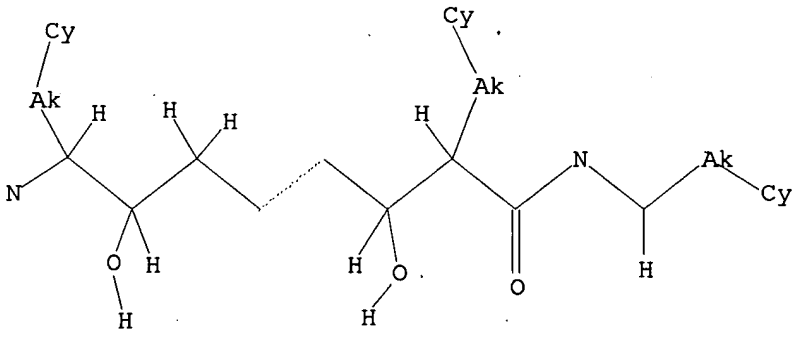
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10683756-1.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:55:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6820 TO ITERATE

29.3% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 131449 TO 141351
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 14:55:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 135643 TO ITERATE

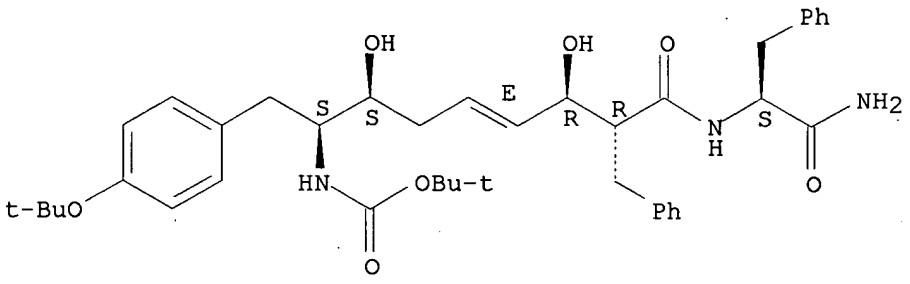
100.0% PROCESSED 135643 ITERATIONS 48 ANSWERS
SEARCH TIME: 00.00.08

L3 48 SEA SSS FUL L1

=> d l3 scan

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Carbamic acid, [(1S,2S,4E,6R,7R)-8-[[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]amino]-1-[[4-(1,1-dimethylethoxy)phenyl]methyl]-2,6-dihydroxy-8-oxo-7-(phenylmethyl)-4-octenyl]-, 1,1-dimethylethyl ester (9CI)
MF C40 H53 N3 O7

Absolute stereochemistry.
Double bond geometry as shown.

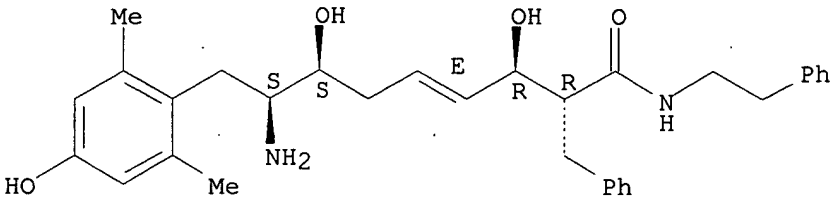


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI)
MF C32 H40 N2 O4

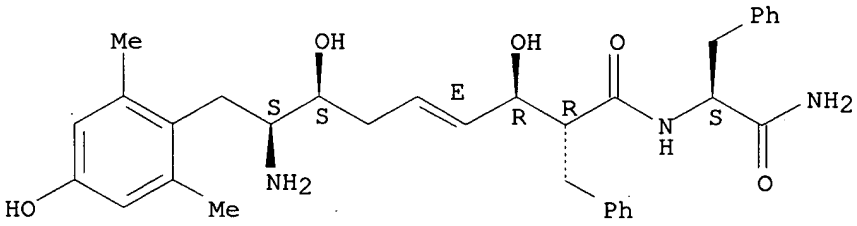
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C33 H41 N3 O5

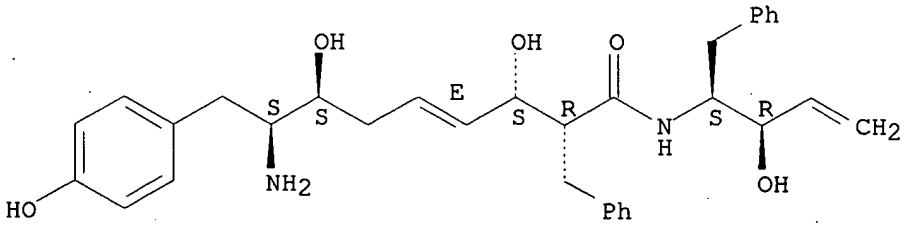
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-butenyl]-, (αR)- (9CI)
MF C33 H40 N2 O5

Absolute stereochemistry.
Double bond geometry as shown.

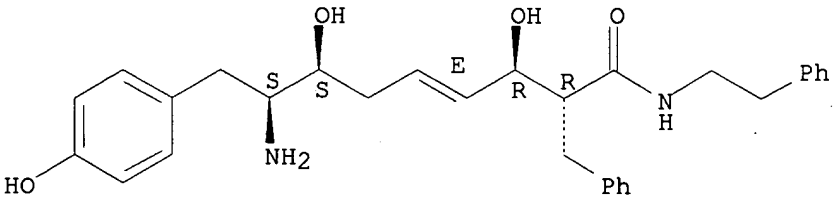


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI)

MF C30 H36 N2 O4

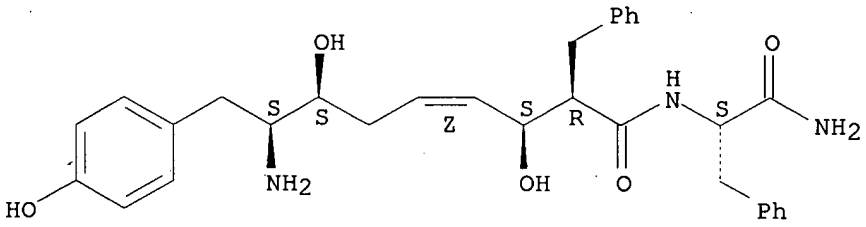
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2Z,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C31 H37 N3 O5

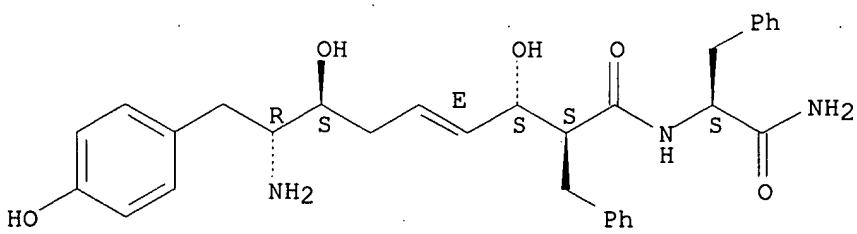
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI)
MF C31 H37 N3 O5

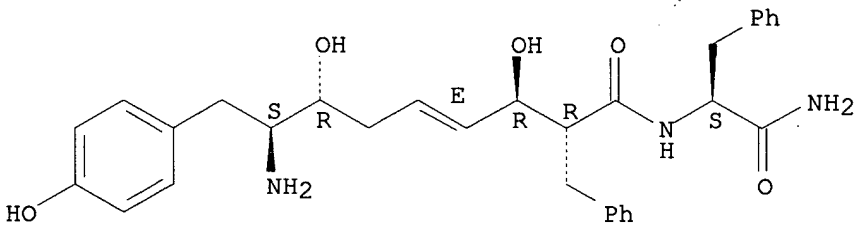
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C31 H37 N3 O5

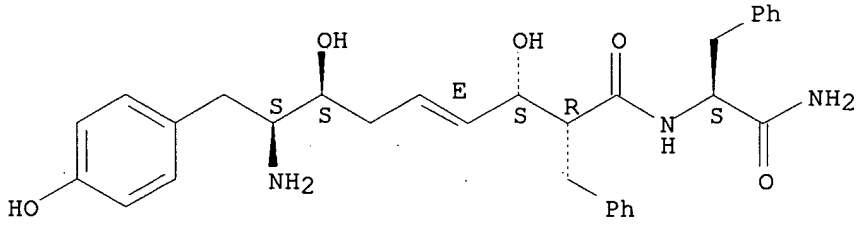
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C31 H37 N3 O5

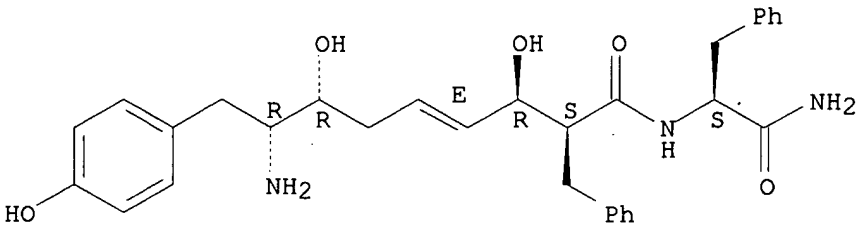
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI)
MF C31 H37 N3 O5

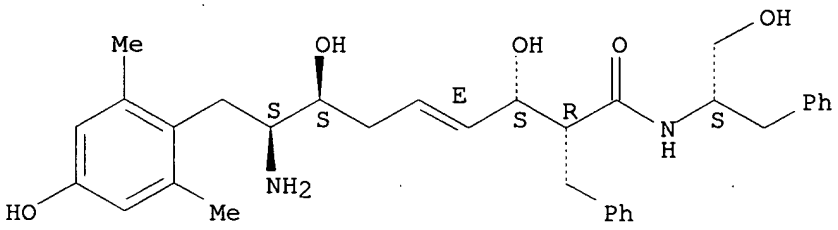
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI)
MF C33 H42 N2 O5

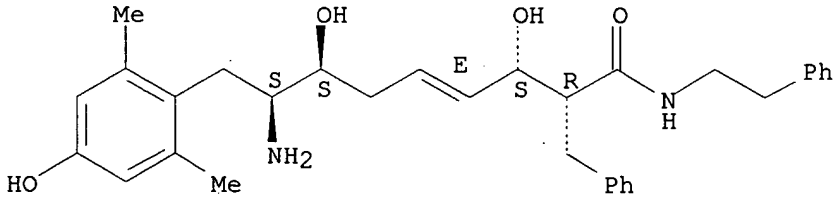
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI)
MF C32 H40 N2 O4

Absolute stereochemistry.
Double bond geometry as shown.

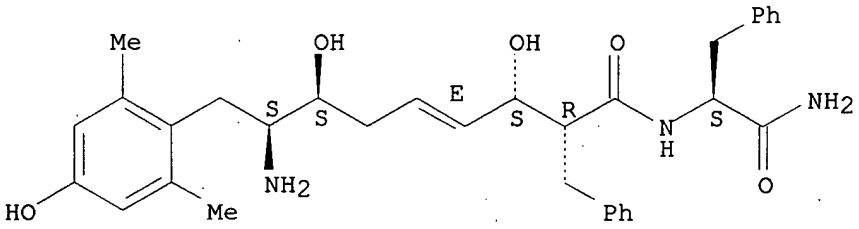


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-

(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C33 H41 N3 O5

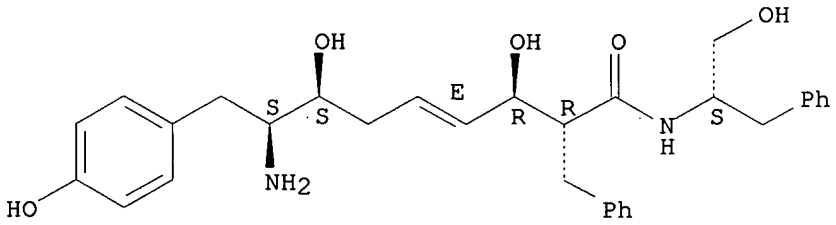
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI)
MF C31 H38 N2 O5

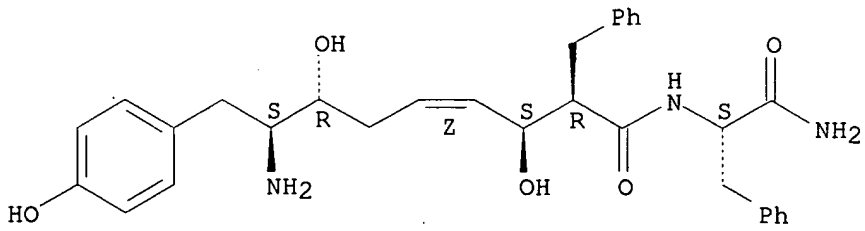
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2Z,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C31 H37 N3 O5

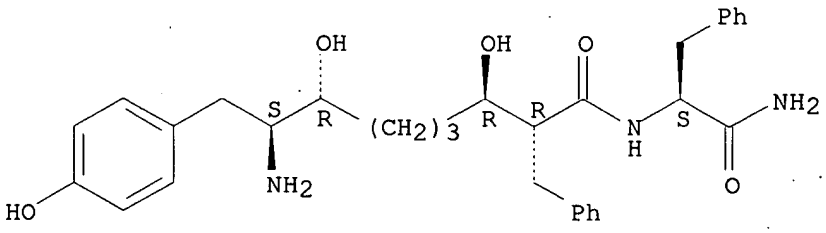
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βR,ζR,ηS)- (9CI)
MF C31 H39 N3 O5

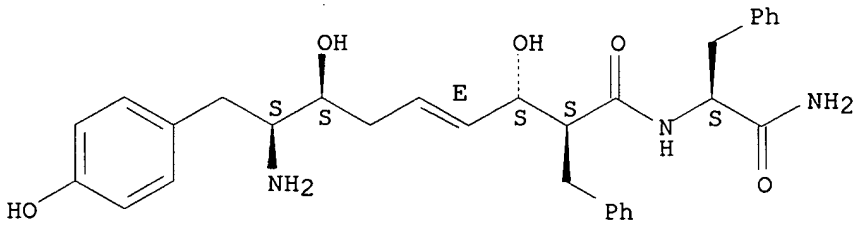
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI)
MF C31 H37 N3 O5

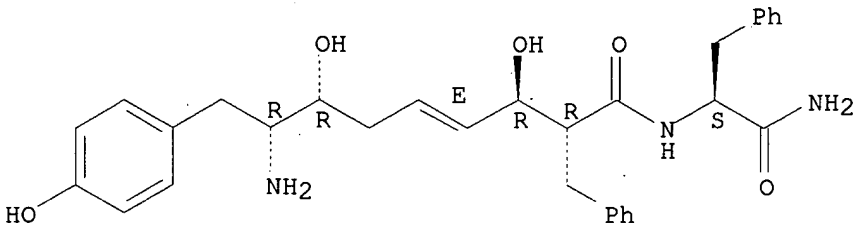
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C31 H37 N3 O5

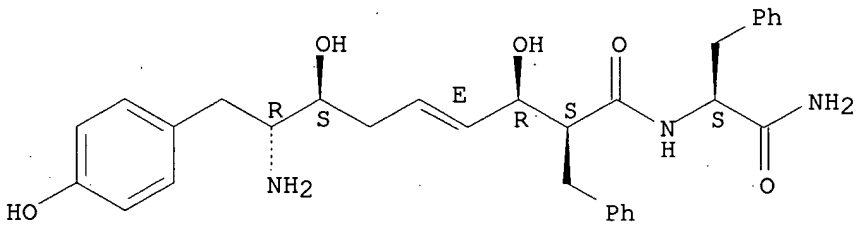
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI)
MF C31 H37 N3 O5

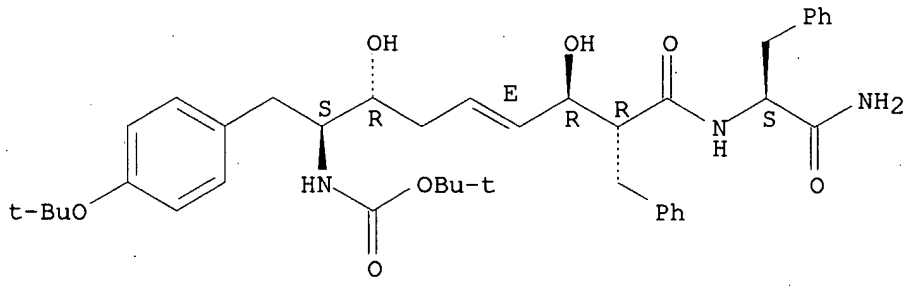
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Carbamic acid, [(1S,2R,4E,6R,7R)-8-[[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]amino]-1-[[4-(1,1-dimethylethoxy)phenyl]methyl]-2,6-dihydroxy-8-oxo-7-(phenylmethyl)-4-octenyl]-, 1,1-dimethylethyl ester (9CI)
MF C40 H53 N3 O7

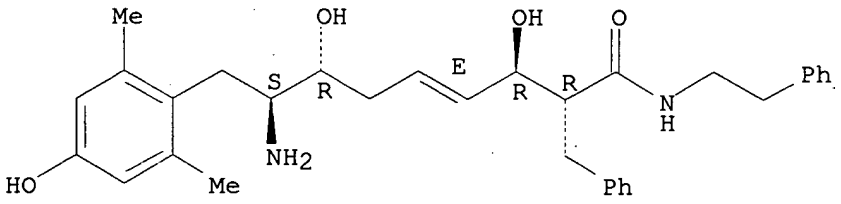
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI)
MF C32 H40 N2 O4

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):o
'O' IS NOT VALID HERE

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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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L4 3 L3

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L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:333687 CAPLUS
DOCUMENT NUMBER: 140:339637
TITLE: Preparation of peptidomimetic μ-opioid receptor ligands
INVENTOR(S): Harrison, Bryce; Gierasch, Tiffany Malinky; Verdine, Gregory L.; Shi, Zhangjie
PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA
SOURCE: PCT Int. Appl., 128 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004033414	A1	20040422	WO 2003-US32280		20031010
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2003279953	A1	20040504	AU 2003-279953		20031010
US 2004254225	A1	20041216	US 2003-683756		20031010
PRIORITY APPLN. INFO.:			US 2002-417925P	P	20021011
			US 2003-443428P	P	20030129
			WO 2003-US32280	W	20031010

OTHER SOURCE(S): MARPAT 140:339637
AB The invention relates to peptidomimetic compds. derived from aralkyl-substituted aminodihydroxyalk(en)oic acids which are modulators of the μ-opioid receptor (MOR) and thus have therapeutic applications. The claims include compds. of general formula R52NCHR1CH(OH)CH2CHRCHRCH(OH)CHR2CO-X-CHR3R4 [R2 is H2 or a bond; X is N, O or S; R1-R3 are (un)substituted (hetero)arylalkyl; R4 is H, CONR72 (R7 is H, alkyl, acyl or a protecting group), CONHR7, CH2OH, CH(OH)CH:CH2 or CONHCHR10CO2H (R10 is an amino acid side chain); R5 is H, alk(en)yl, (hetero)aryl, acyl, a protecting group or COCHR10CO2H] or their pharmaceutically-acceptable salts. Thus, stereoisomeric H2NCH(CH2C6H4OH-p)CH(OH)CH2CH:CHCH(OH)CH(CH2Ph)CONHCH(CH2Ph)CONH2 (2) were prepared and assayed for binding affinity for MOR [8.8 ± 0.7 nM for (S,S,S,R)-2, vs. 1.2 ± 0.1 nM for endomorphin 2].
IT 479495-67-5P 479495-68-6P 479495-69-7P
479495-70-0P 479495-71-1P 479495-72-2P
479495-73-3P 479495-74-4P 479495-75-5P
479495-76-6P 479495-77-7P 479495-78-8P
479495-79-9P 479495-80-2P 479495-81-3P
479495-83-5P 479495-84-6P 479495-85-7P
479495-86-8P 479496-03-2P 479496-04-3P
479496-05-4P 479496-06-5P 479496-11-2P
479496-12-3P 479496-13-4P 479496-14-5P
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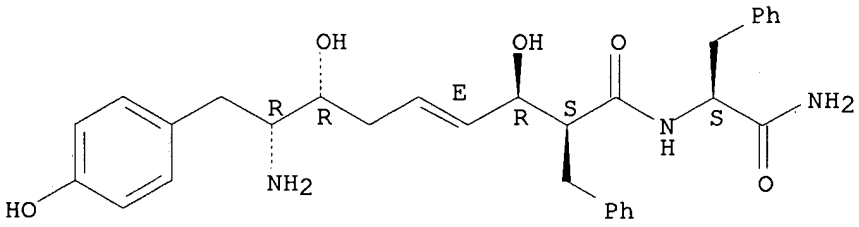
479496-18-9P 479496-19-0P 503186-38-7P
503186-39-8P 503186-40-1P 503186-41-2P

503186-42-3P 503186-43-4P 503186-44-5P
503186-45-6P 503186-46-7P 503186-47-8P
503186-48-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidomimetic μ-opioid receptor ligands)

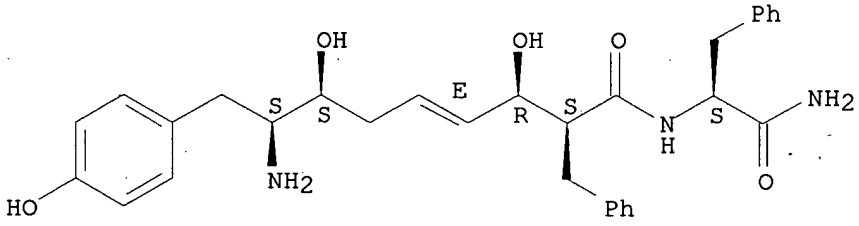
RN 479495-67-5 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



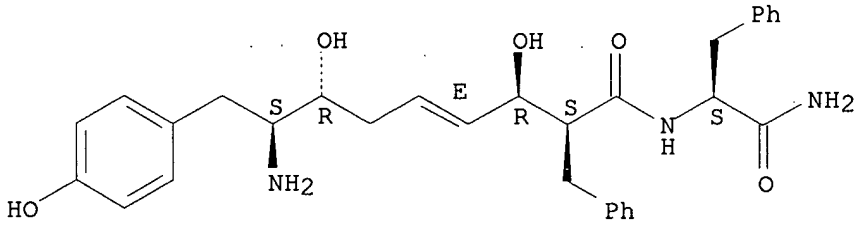
RN 479495-68-6 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 479495-69-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

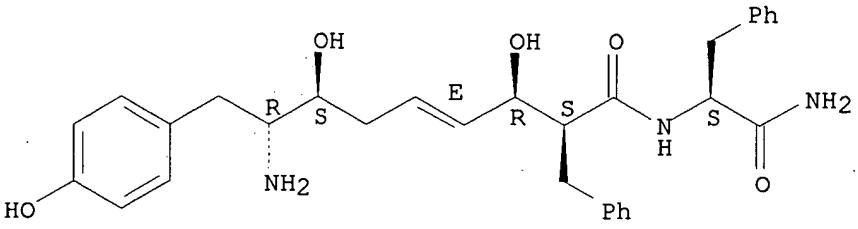
Absolute stereochemistry.
Double bond geometry as shown.



RN 479495-70-0 CAPLUS

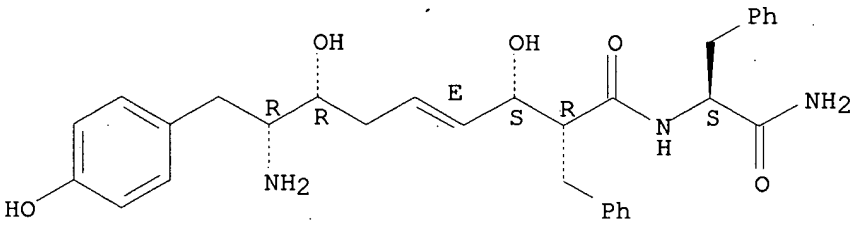
CN Benzenepropanamide, α-[(1R,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



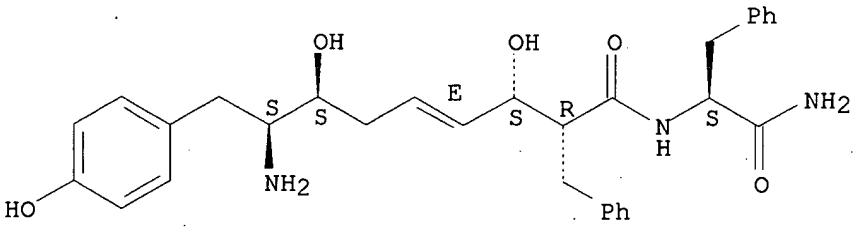
RN 479495-71-1 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



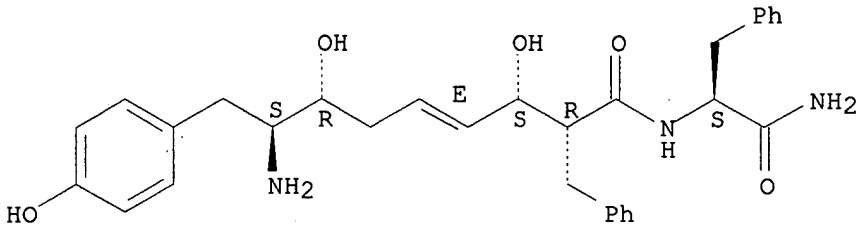
RN 479495-72-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



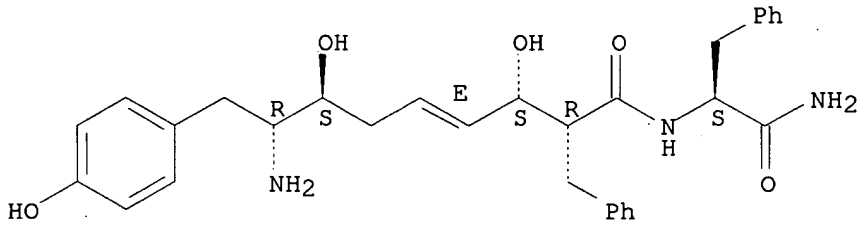
RN 479495-73-3 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



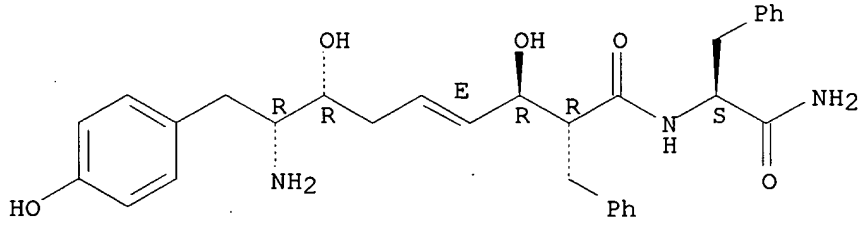
RN 479495-74-4 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



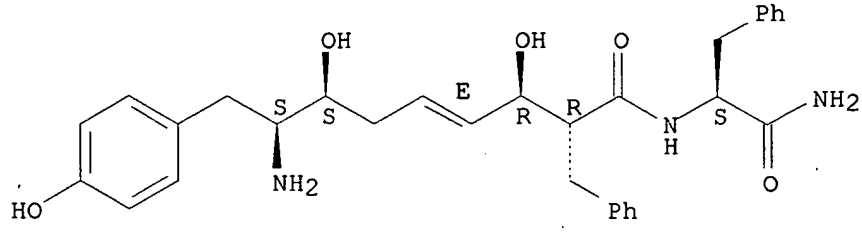
RN 479495-75-5 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



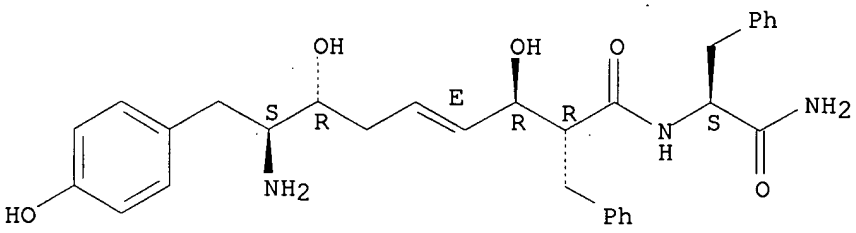
RN 479495-76-6 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



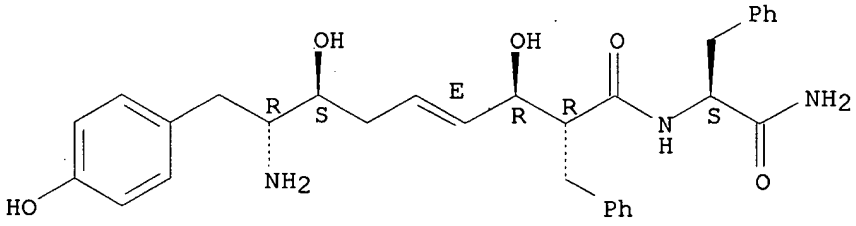
RN 479495-77-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



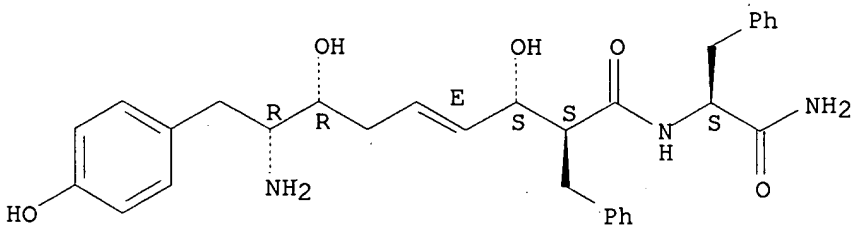
RN 479495-78-8 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



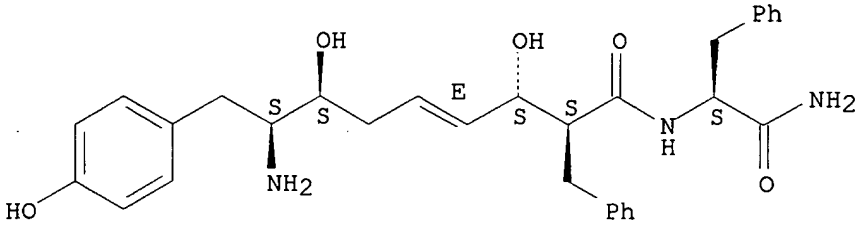
RN 479495-79-9 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



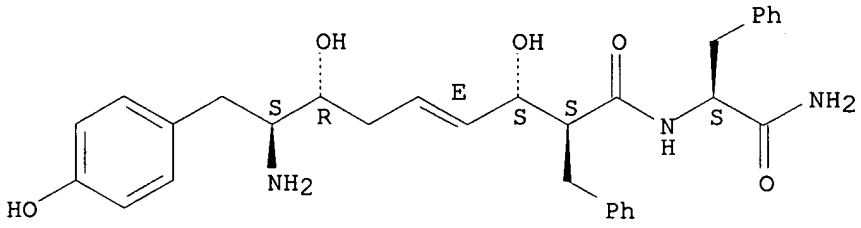
RN 479495-80-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



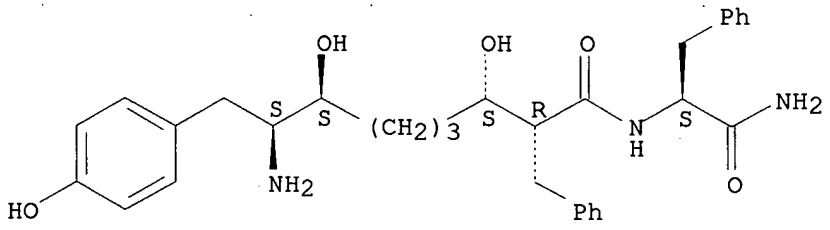
RN 479495-81-3 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



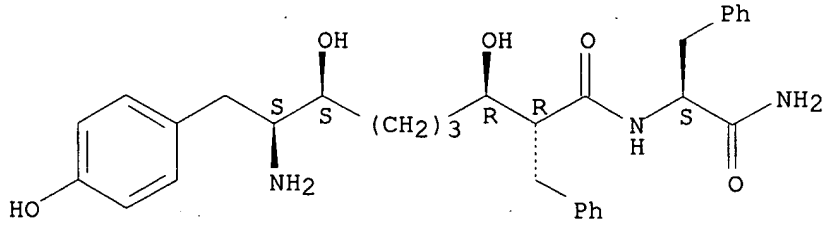
RN 479495-83-5 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βS,ζS,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



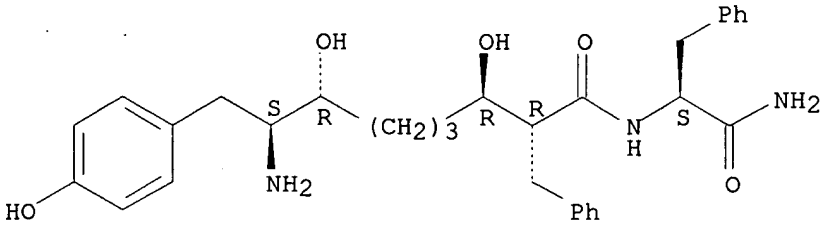
RN 479495-84-6 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βR,ζS,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



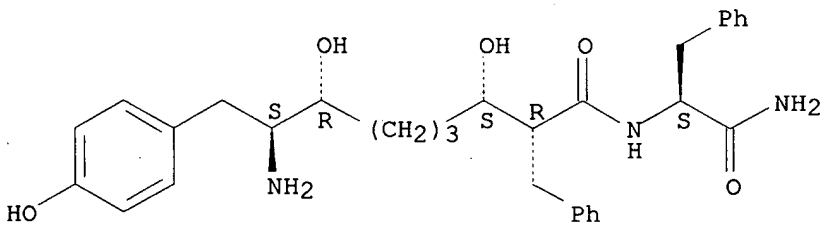
RN 479495-85-7 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βR,ζR,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



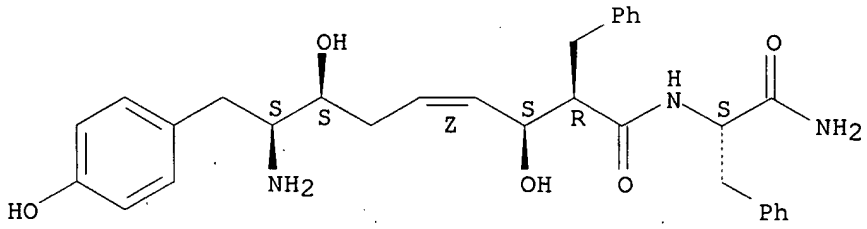
RN 479495-86-8 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βS,ζR,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



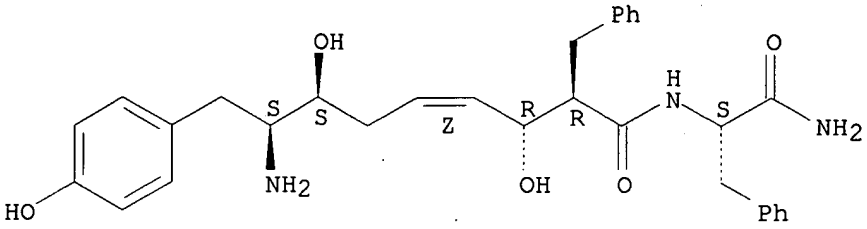
RN 479496-03-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2Z,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



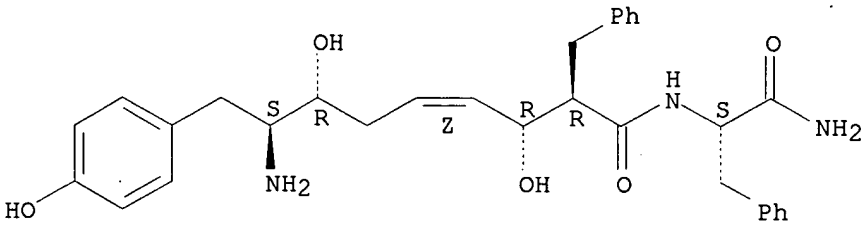
RN 479496-04-3 CAPLUS
CN Benzenepropanamide, α-[(1R,2Z,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



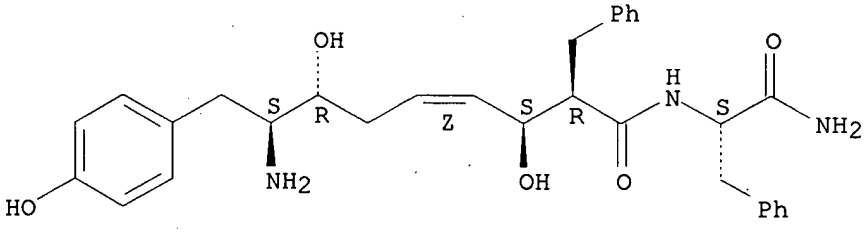
RN 479496-05-4 CAPLUS
CN Benzenepropanamide, α-[(1R,2Z,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



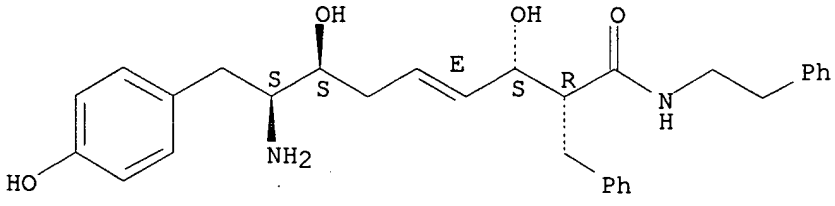
RN 479496-06-5 CAPLUS
CN Benzenepropanamide, α-[(1S,2Z,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



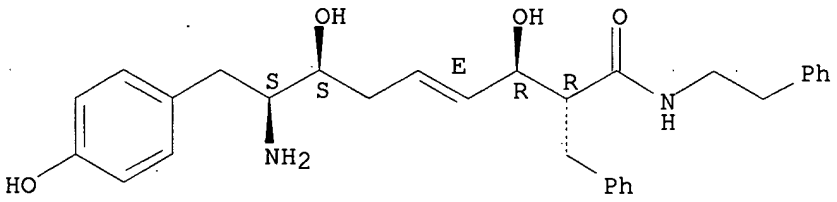
RN 479496-11-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



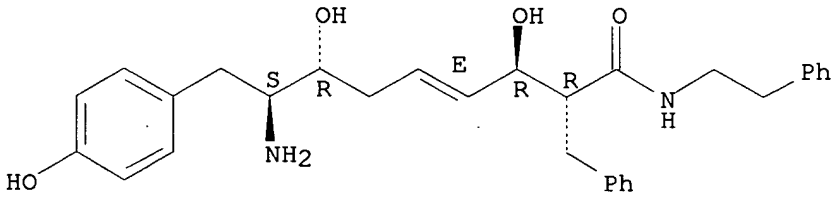
RN 479496-12-3 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



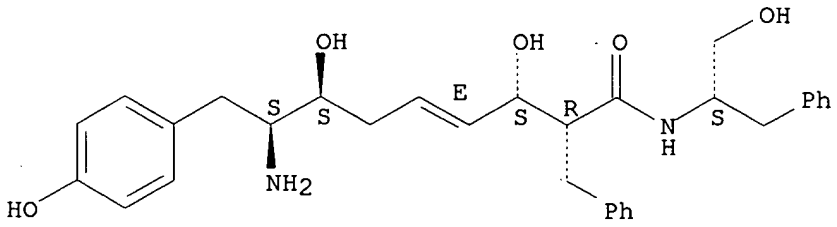
RN 479496-13-4 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



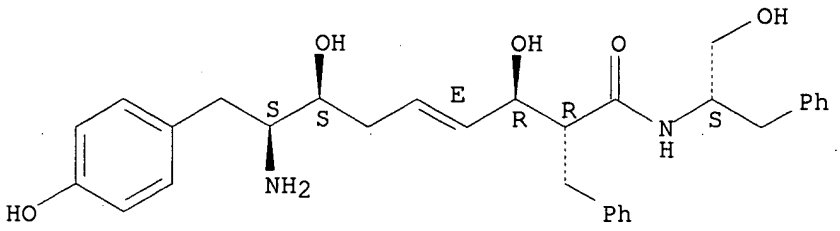
RN 479496-14-5 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



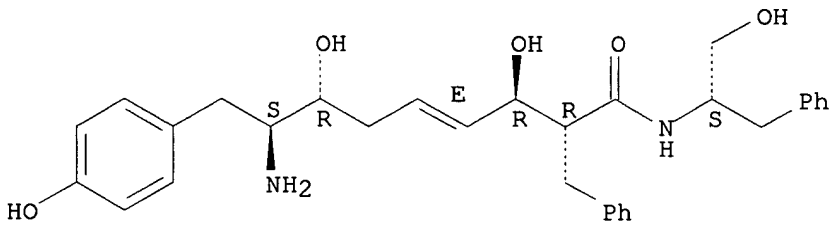
RN 479496-15-6 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



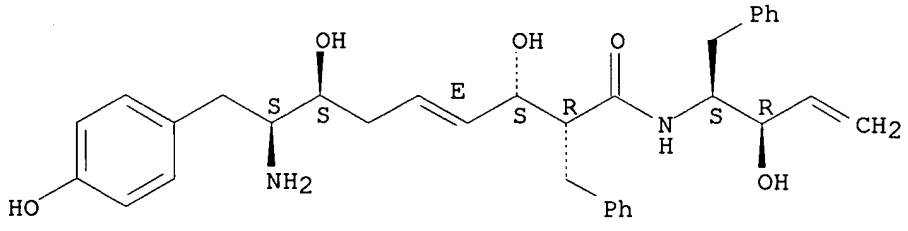
RN 479496-16-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



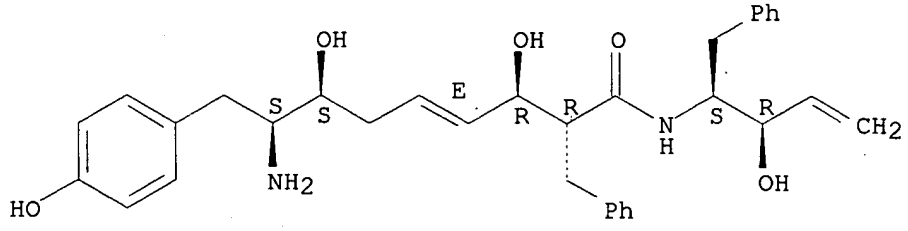
RN 479496-17-8 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-butenyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



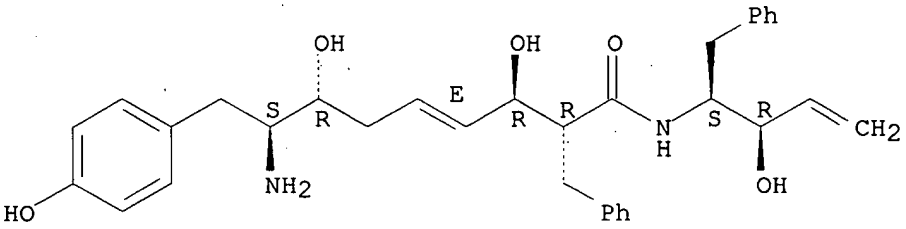
RN 479496-18-9 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-butenyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



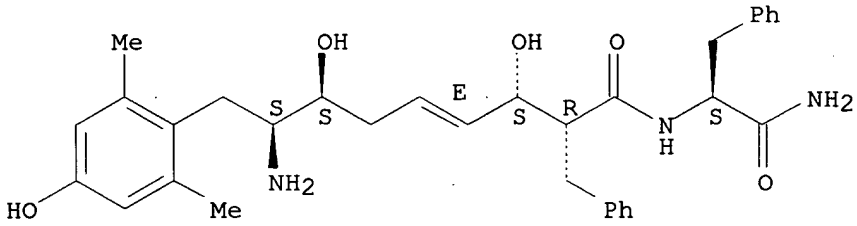
RN 479496-19-0 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-butenyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



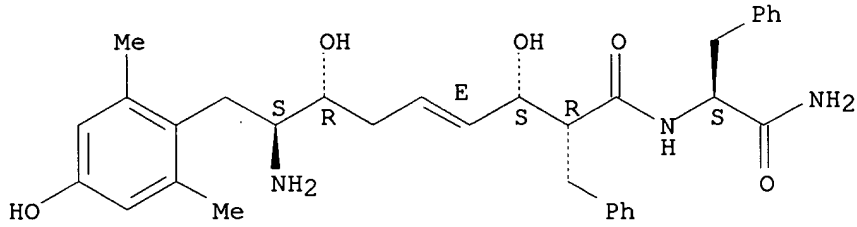
RN 503186-38-7 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



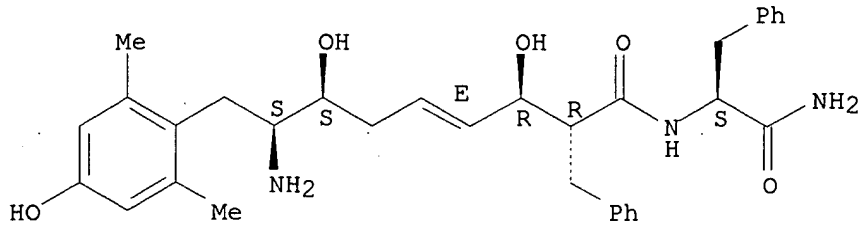
RN 503186-39-8 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



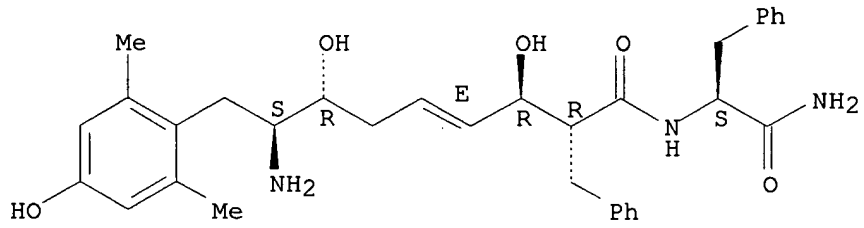
RN 503186-40-1 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



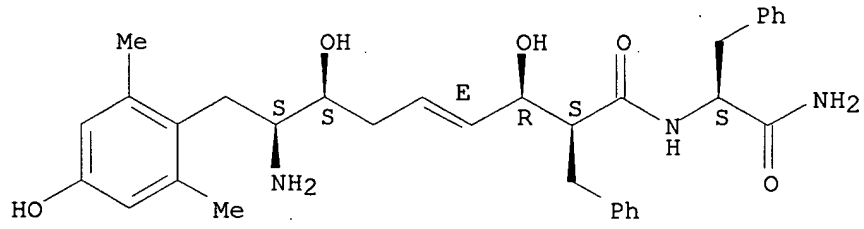
RN 503186-41-2 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



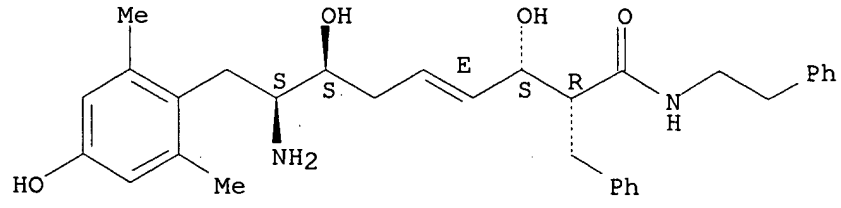
RN 503186-42-3 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



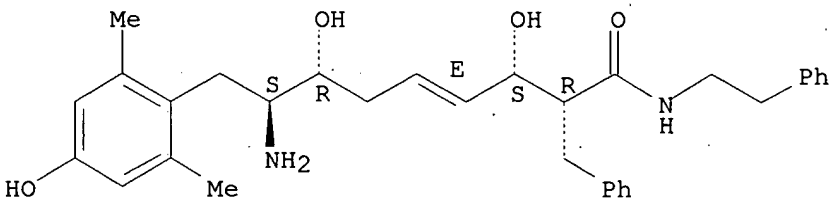
RN 503186-43-4 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



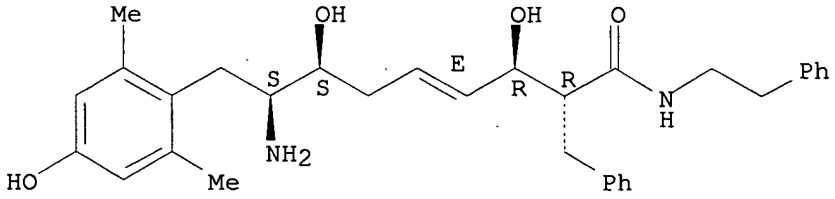
RN 503186-44-5 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



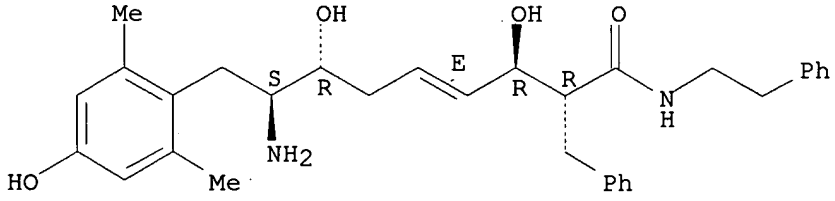
RN 503186-45-6 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



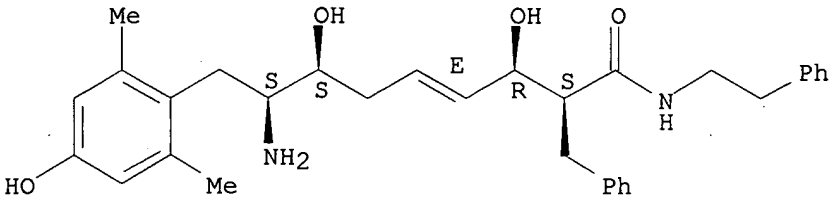
RN 503186-46-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



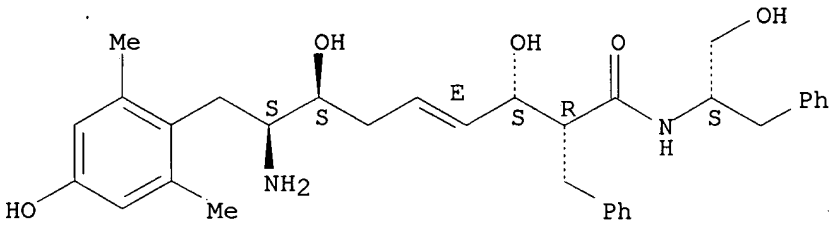
RN 503186-47-8 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



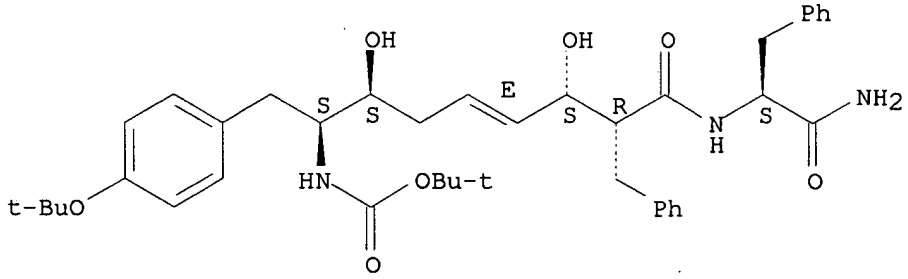
RN 503186-48-9 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



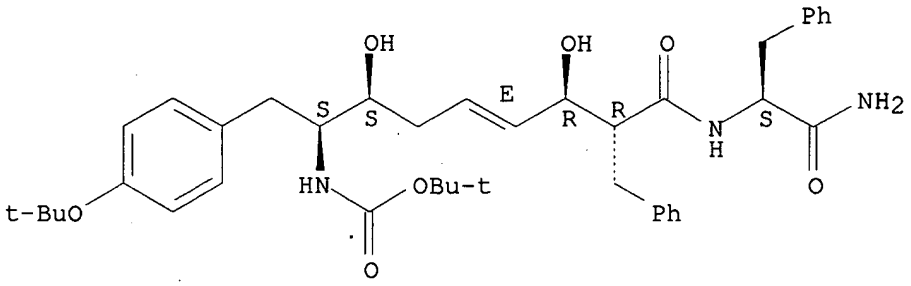
IT 680187-48-8DP, resin-bound 680187-49-9DP, resin-bound
680187-50-2DP, resin-bound 680187-51-3DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidomimetic μ-opioid receptor ligands)
RN 680187-48-8 CAPLUS
CN Carbamic acid, [(1S,2S,4E,6S,7R)-8-[[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]amino]-1-[[4-(1,1-dimethylethoxy)phenyl]methyl]-2,6-dihydroxy-8-oxo-7-(phenylmethyl)-4-octenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



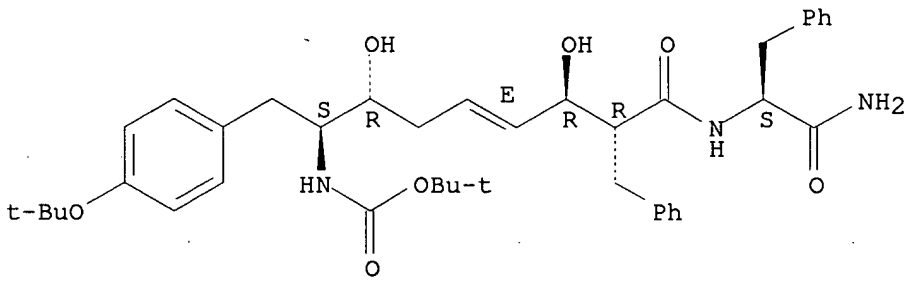
RN 680187-49-9 CAPLUS
CN Carbamic acid, [(1S,2S,4E,6R,7R)-8-[[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]amino]-1-[[4-(1,1-dimethylethoxy)phenyl]methyl]-2,6-dihydroxy-8-oxo-7-(phenylmethyl)-4-octenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



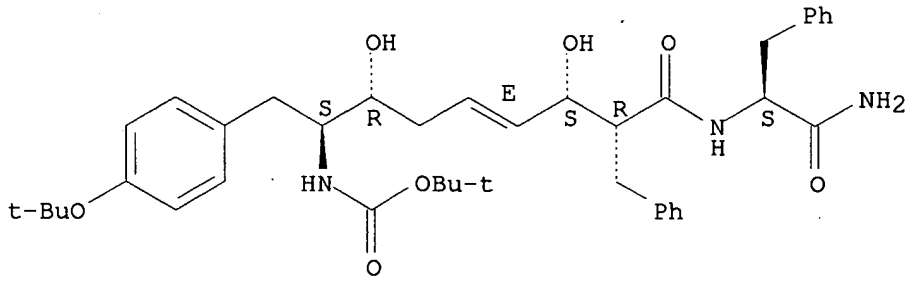
RN 680187-50-2 CAPLUS
CN Carbamic acid, [(1S,2R,4E,6R,7R)-8-[[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]amino]-1-[[4-(1,1-dimethylethoxy)phenyl]methyl]-2,6-dihydroxy-8-oxo-7-(phenylmethyl)-4-octenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 680187-51-3 CAPLUS
CN Carbamic acid, [(1S,2R,4E,6S,7R)-8-[[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]amino]-1-[[4-(1,1-dimethylethoxy)phenyl]methyl]-2,6-dihydroxy-8-oxo-7-(phenylmethyl)-4-octenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

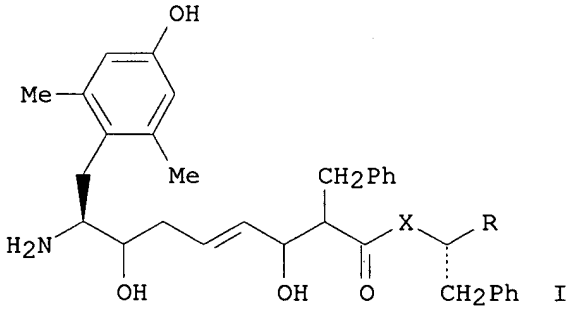
L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:72698 CAPLUS
DOCUMENT NUMBER: 138:271935
TITLE: 2,6-Dimethyltyrosine Analogues of a Stereodiversified Ligand Library: Highly Potent, Selective, Non-Peptidic

μ Opioid Receptor Agonists

AUTHOR(S): Harrison, Bryce A.; Pasternak, Gavril W.; Verdine, Gregory L.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SOURCE: Journal of Medicinal Chemistry (2003), 46(5), 677-680
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:271935

GI



I

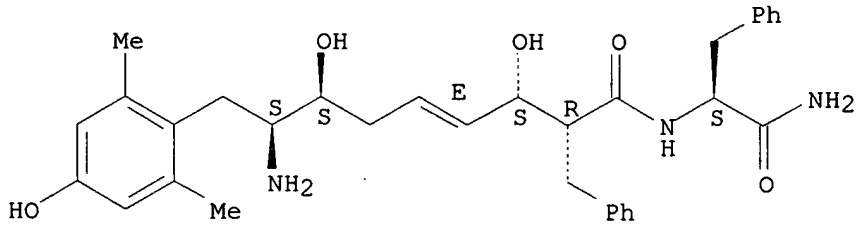
AB The authors report the synthesis and bioactivity of enediol-based 2,6-dimethyltyrosine analogs I (X = NH, R = CONH2; X = NH, R = H; X = NH, R = CH2OH; X = O, R = CONH2; X = O, R = H; X = O, R = CH2OH) towards μ-opioid receptor. For I (X = NH, R = CONH2; X = NH, R = H), five stereoisomers of each compound were synthesized and their bioactivity evaluated, discovering certain stereoisomers with unexpected potency, selectivity, and efficacy.

IT 503186-38-7P 503186-39-8P 503186-40-1P
503186-41-2P 503186-42-3P 503186-43-4P
503186-44-5P 503186-45-6P 503186-46-7P
503186-47-8P 503186-48-9P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(asym. preparation of enediol-based nonpeptidic analogs of dimethyltyrosine and their evaluation as μ-opioid receptor agonists)

RN 503186-38-7 CAPLUS

CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

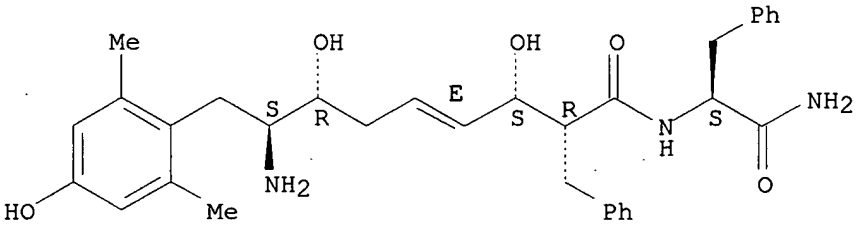
Absolute stereochemistry.
Double bond geometry as shown.



RN 503186-39-8 CAPLUS

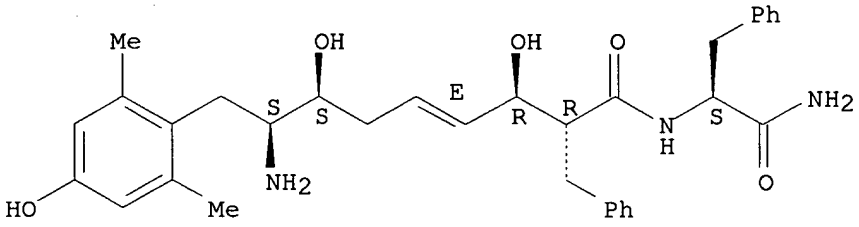
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



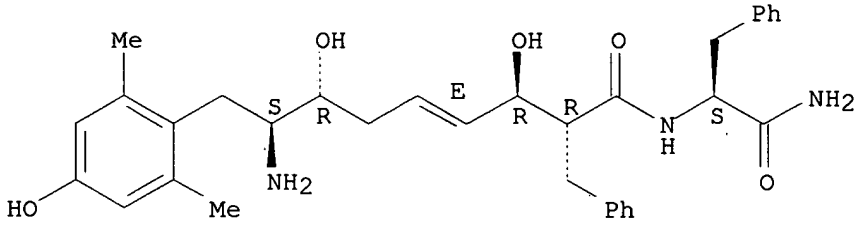
RN 503186-40-1 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



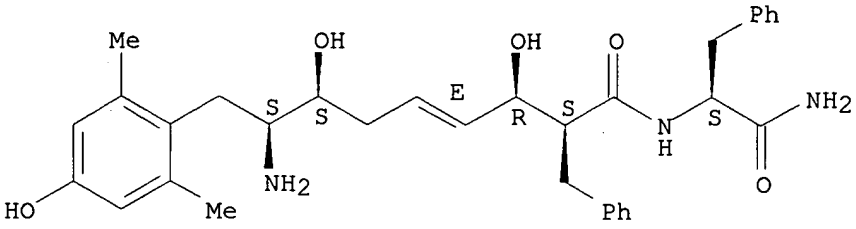
RN 503186-41-2 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



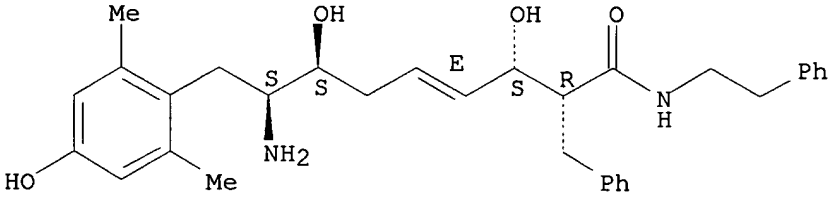
RN 503186-42-3 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



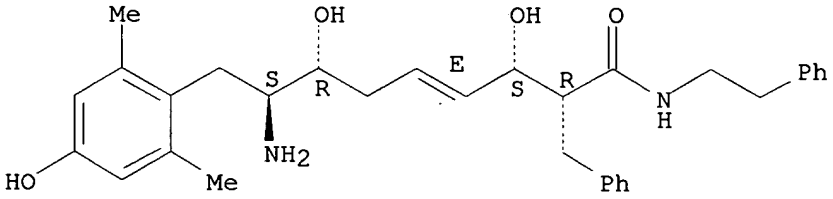
RN 503186-43-4 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



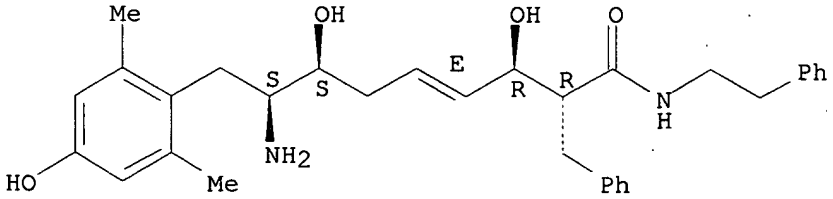
RN 503186-44-5 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 503186-45-6 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)-(9CI) (CA INDEX NAME)

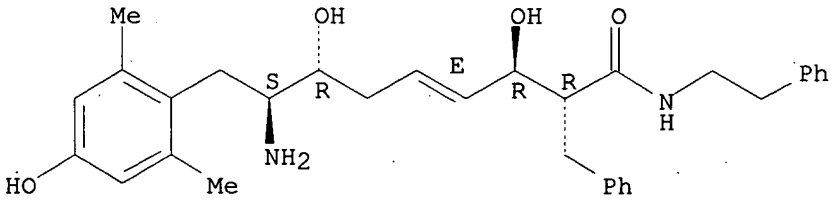
Absolute stereochemistry.
Double bond geometry as shown.



RN 503186-46-7 CAPLUS

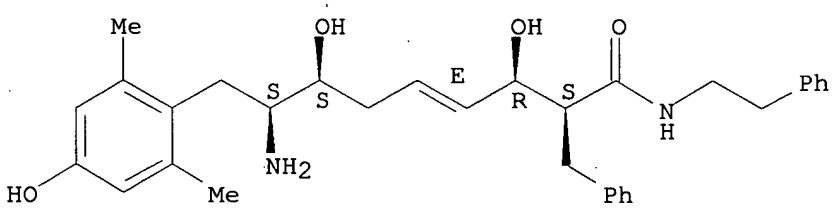
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



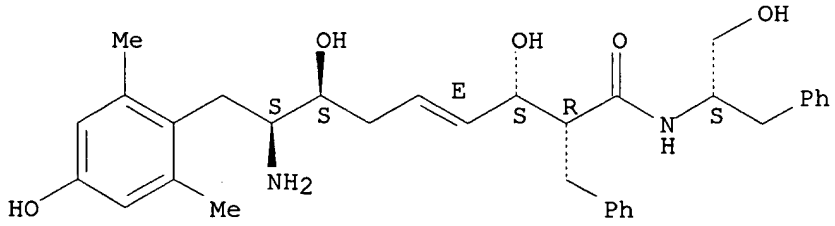
RN 503186-47-8 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 503186-48-9 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

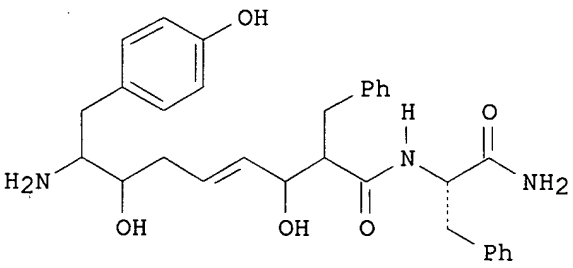
Absolute stereochemistry.
Double bond geometry as shown.



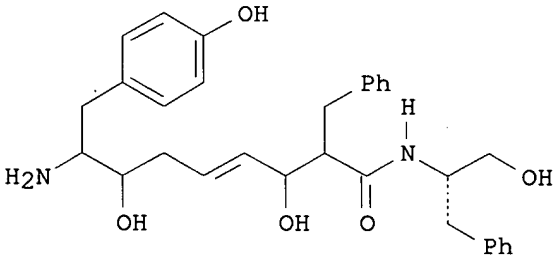
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:808520 CAPLUS
DOCUMENT NUMBER: 138:55660
TITLE: High-Affinity Mu Opioid Receptor Ligands Discovered by the Screening of an Exhaustively Stereodiversified Library of 1,5-Enediols
AUTHOR(S): Harrison, Bryce A.; Gierasch, Tiffany Malinky; Neilan, Claire; Pasternak, Gavril W.; Verdine, Gregory L.

CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (2002), 124(45), 13352-13353
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:55660
GI



I



II

AB A stereodiversified library of all 16 stereoisomers of 1,5-enediol I was synthesized, and these compds. were screened for mu opioid receptor (MOR) binding. The stereochem. configuration of I strongly impacted the binding affinity, and (S,S,S,R)-I exhibited a Ki of 8.8 nM for MOR, comparable to that of endomorphin-2 (Ki = 1.2 nM). Moreover, compds. I exhibited 5-86-fold selectivity for MOR over delta opioid receptor (DOR) and 16-150-fold selectivity for MOR over kappa opioid receptor (KOR). Addnl., analogs of I were synthesized which showed that the trans configuration of the olefin was important for receptor binding but modifications of the C-terminal amino acid were well tolerated. Of these analogs, tetraols II are noteworthy because they retain only one of the amide bonds present in endomorphin-2, but bind MOR with an affinity of 10 nM and 110- and 600-fold selectivity for MOR over DOR and KOR. These results demonstrate the utility of stereochem. diversity in the discovery of bioactive small mols.

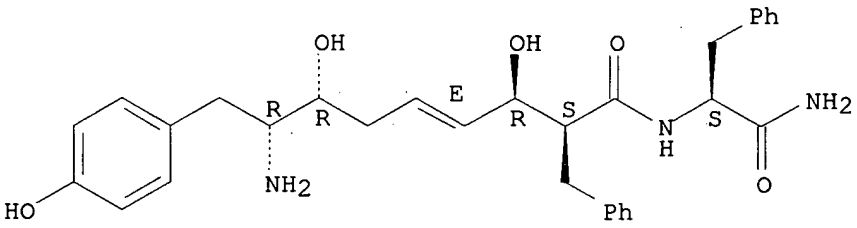
IT 479495-67-5P 479495-68-6P 479495-69-7P
479495-70-0P 479495-71-1P 479495-72-2P
479495-73-3P 479495-74-4P 479495-75-5P
479495-76-6P 479495-77-7P 479495-78-8P
479495-79-9P 479495-80-2P 479495-81-3P
479495-82-4P 479495-83-5P 479495-84-6P
479495-85-7P 479495-86-8P 479496-03-2P
479496-04-3P 479496-05-4P 479496-06-5P
479496-11-2P 479496-12-3P 479496-13-4P
479496-14-5P 479496-15-6P 479496-16-7P
479496-17-8P 479496-18-9P 479496-19-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of amino(dihydroxy)nonenamides and derivs. as nonpeptidic high-affinity μ-opioid receptor ligands)

RN 479495-67-5 CAPLUS

CN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

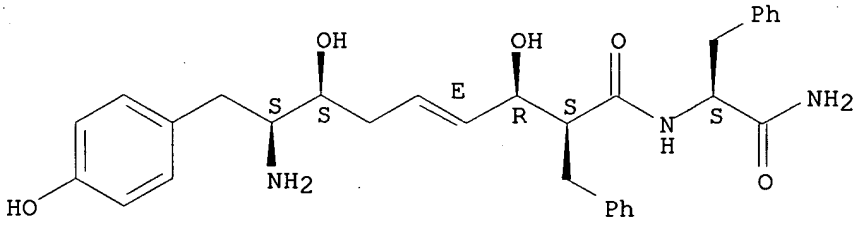
Absolute stereochemistry.
Double bond geometry as shown.



RN 479495-68-6 CAPLUS

CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

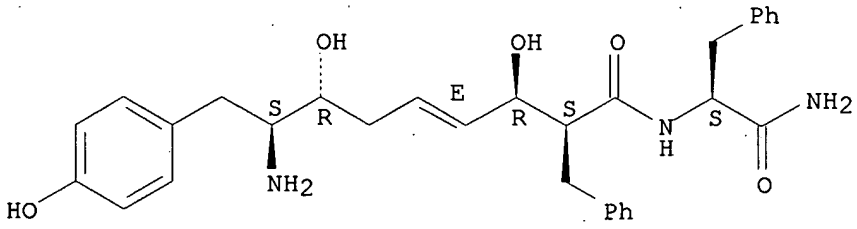
Absolute stereochemistry.
Double bond geometry as shown.



RN 479495-69-7 CAPLUS

CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

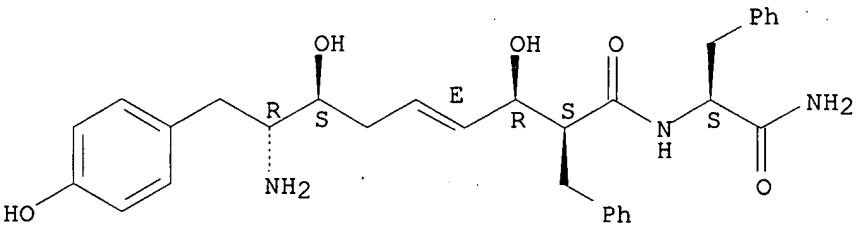
Absolute stereochemistry.
Double bond geometry as shown.



RN 479495-70-0 CAPLUS

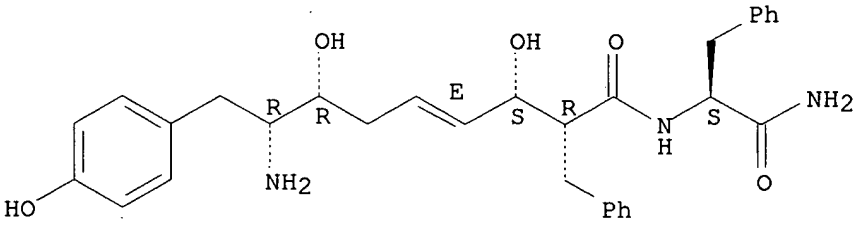
CN Benzenepropanamide, α-[(1R,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



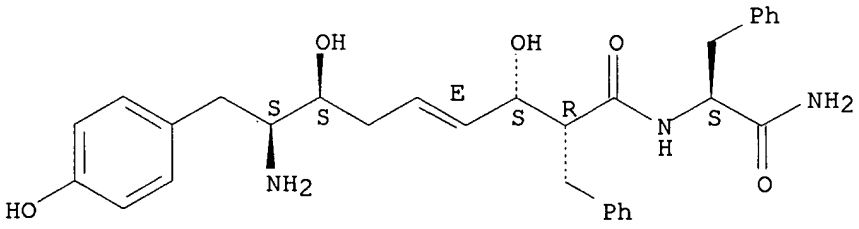
RN 479495-71-1 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



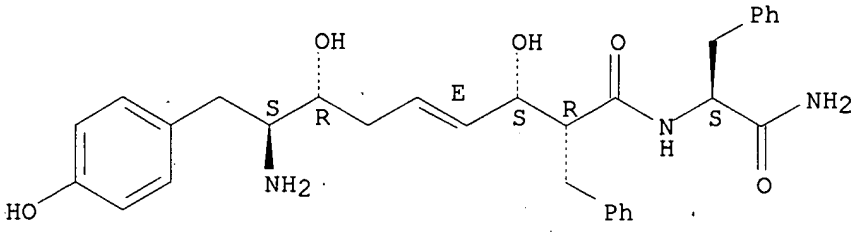
RN 479495-72-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



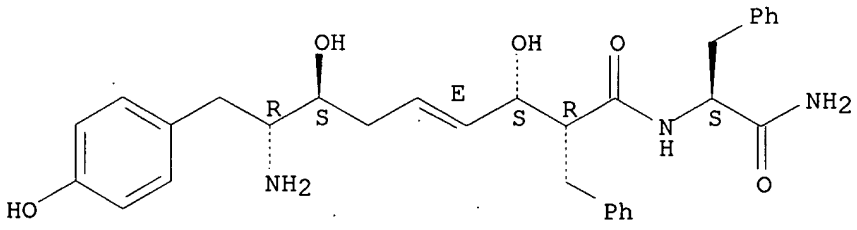
RN 479495-73-3 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



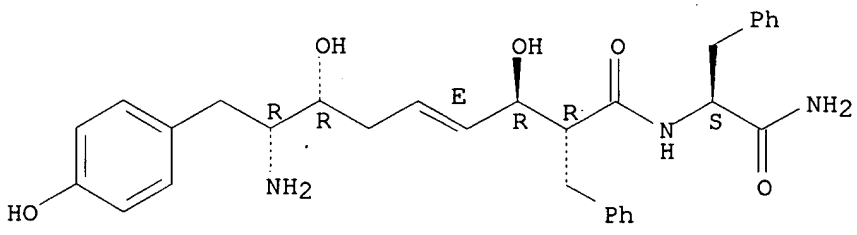
RN 479495-74-4 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



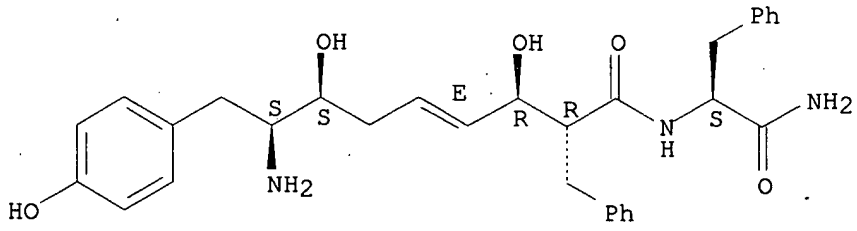
RN 479495-75-5 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



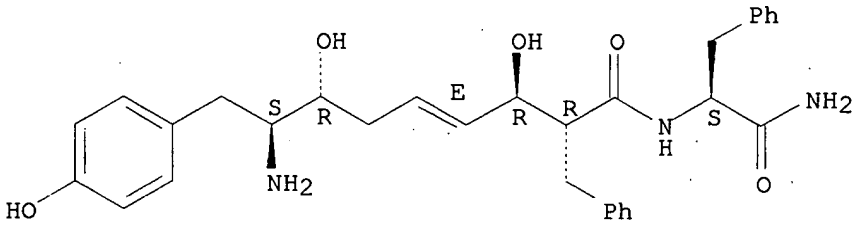
RN 479495-76-6 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



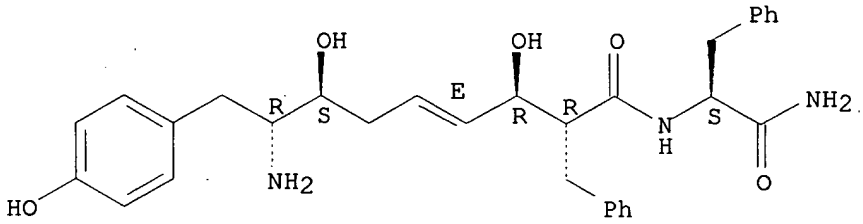
RN 479495-77-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



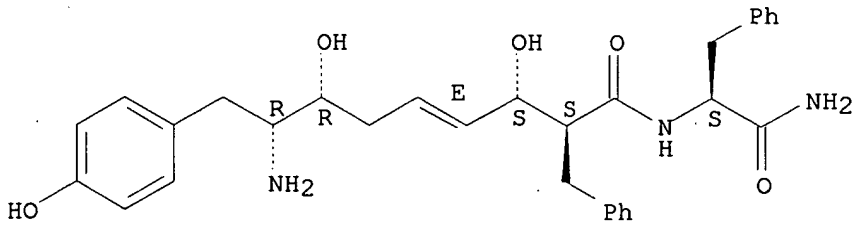
RN 479495-78-8 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



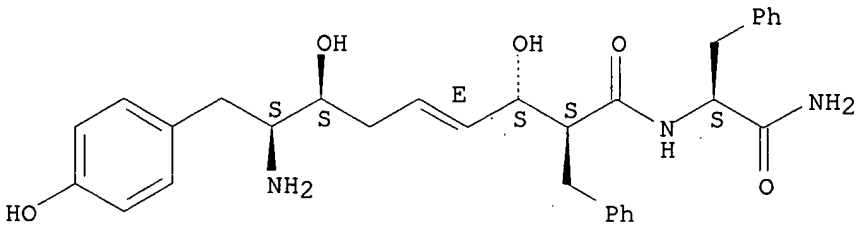
RN 479495-79-9 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



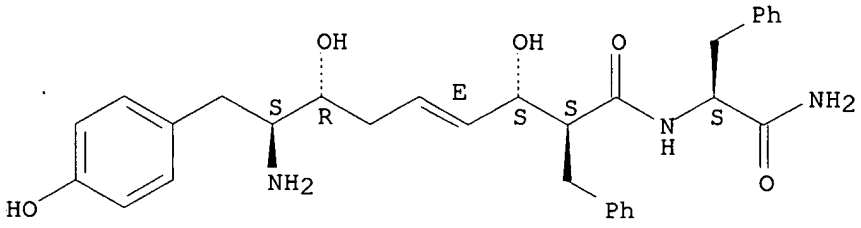
RN 479495-80-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



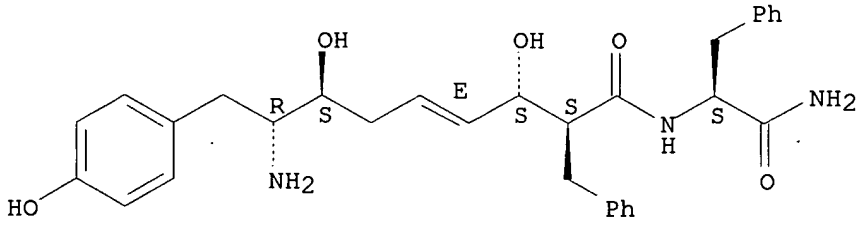
RN 479495-81-3 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



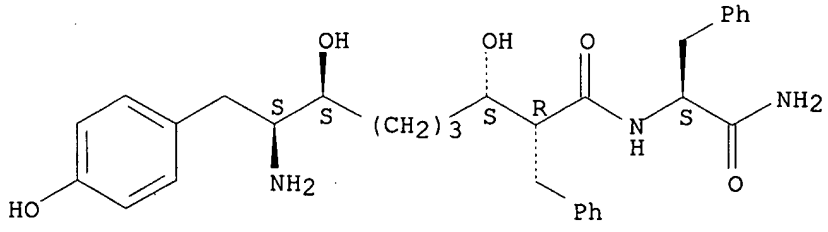
RN 479495-82-4 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



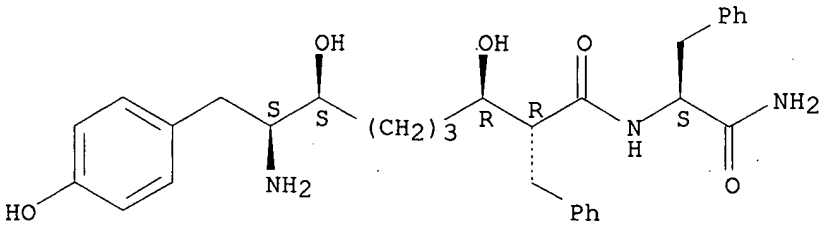
RN 479495-83-5 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βS,ζS,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



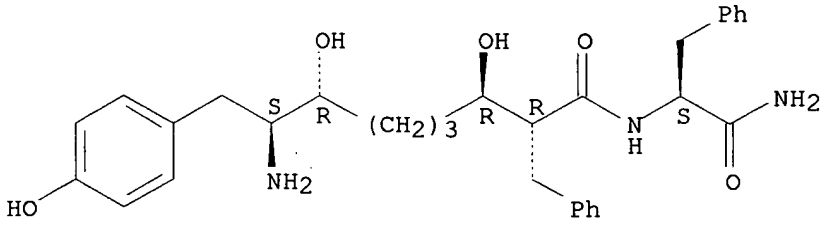
RN 479495-84-6 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βR,ζS,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



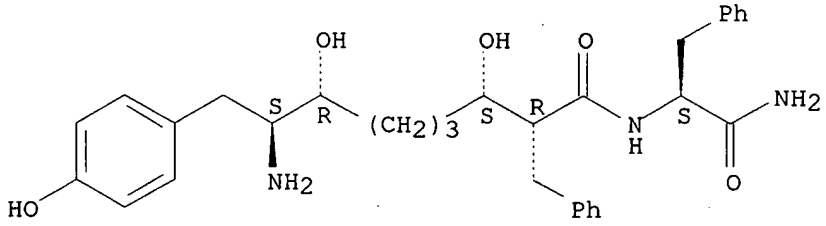
RN 479495-85-7 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βR,ζR,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



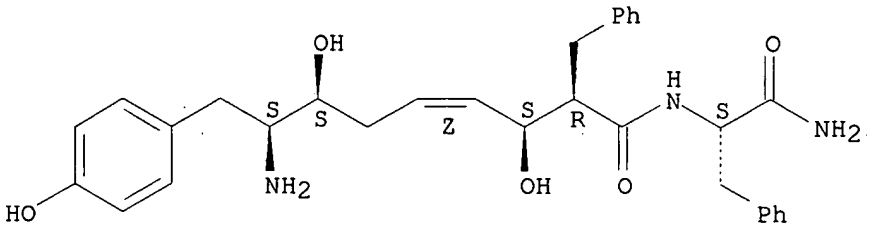
RN 479495-86-8 CAPLUS
CN Benzenenonanamide, η-amino-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-β,ζ,4-trihydroxy-α-(phenylmethyl)-, (αR,βS,ζR,ηS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



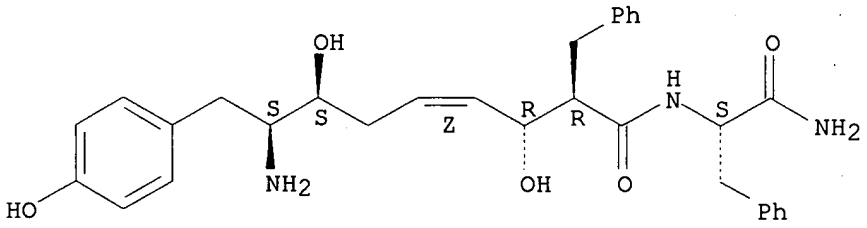
RN 479496-03-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2Z,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



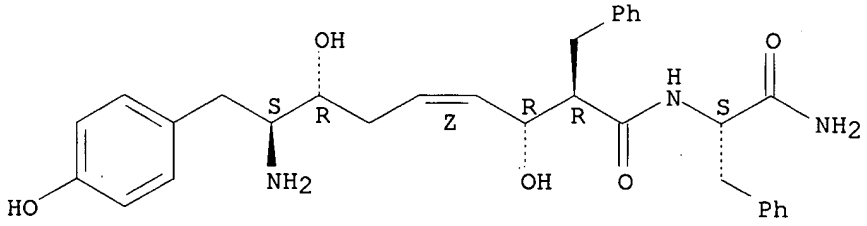
RN 479496-04-3 CAPLUS
CN Benzenepropanamide, α-[(1R,2Z,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



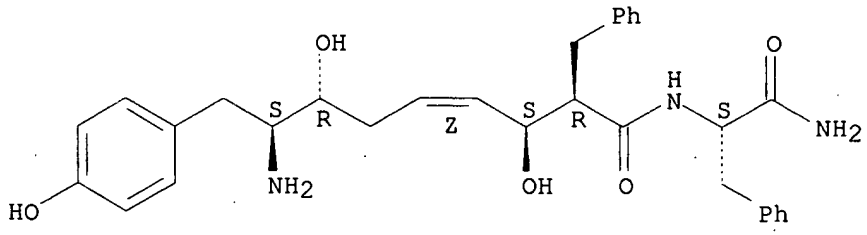
RN 479496-05-4 CAPLUS
CN Benzenepropanamide, α-[(1R,2Z,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



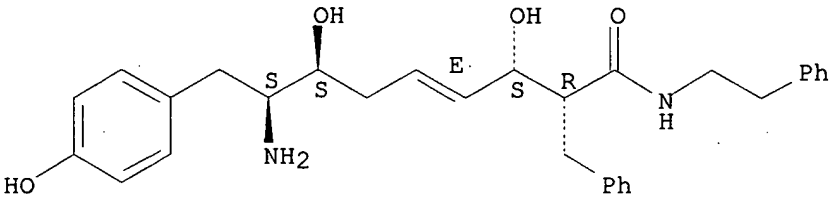
RN 479496-06-5 CAPLUS
CN Benzenepropanamide, α-[(1S,2Z,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



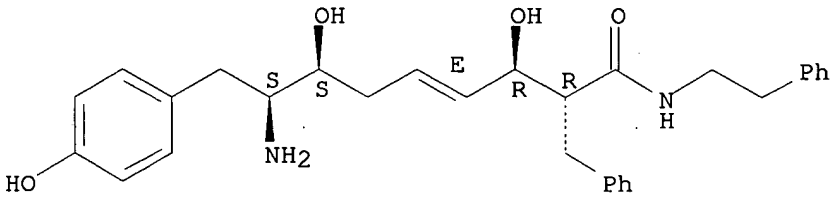
RN 479496-11-2 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



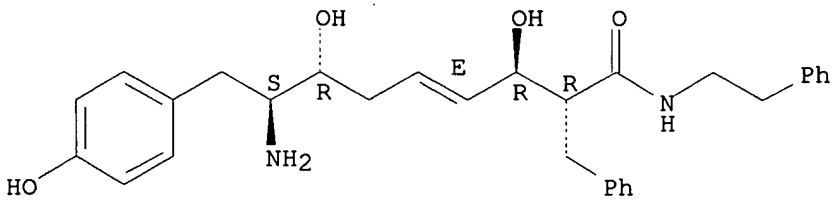
RN 479496-12-3 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



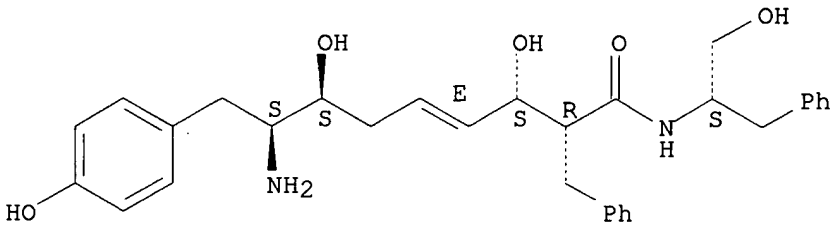
RN 479496-13-4 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-(2-phenylethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



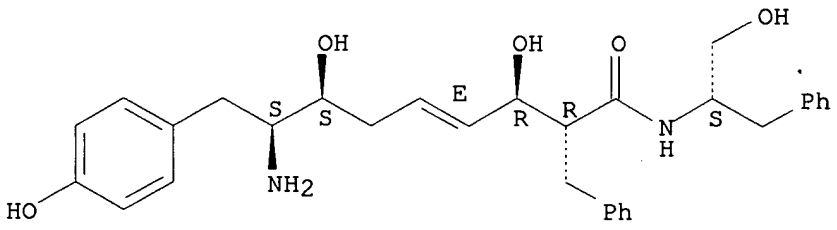
RN 479496-14-5 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



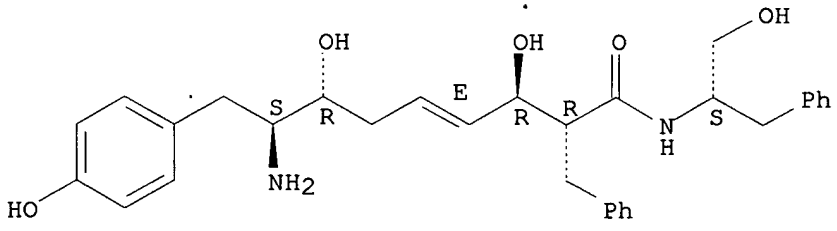
RN 479496-15-6 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



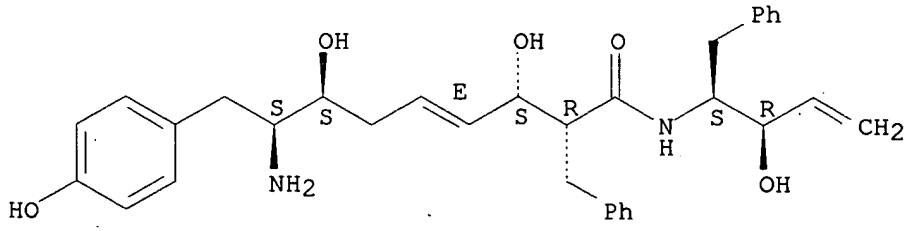
RN 479496-16-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-1-(hydroxymethyl)-2-phenylethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



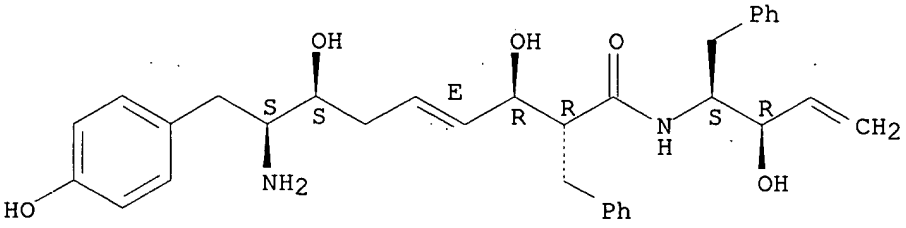
RN 479496-17-8 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-butenyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



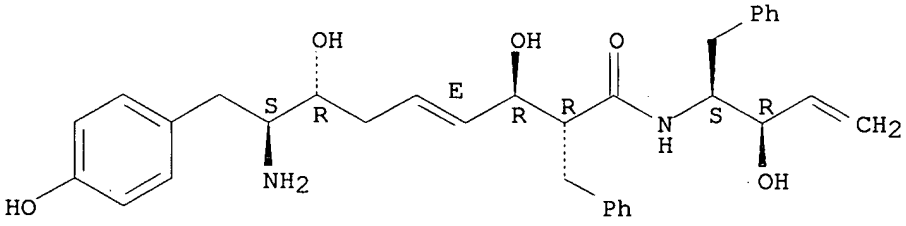
RN 479496-18-9 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-butenyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 479496-19-0 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,5R,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-butenyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.25	183.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

FILE 'STNGUIDE' ENTERED AT 14:57:59 ON 10 NOV 2006

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 3, 2006 (20061103/UP).

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.48	184.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -2.25

FILE 'REGISTRY' ENTERED AT 15:02:34 ON 10 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 NOV 2006 HIGHEST RN 912878-87-6
DICTIONARY FILE UPDATES: 9 NOV 2006 HIGHEST RN 912878-87-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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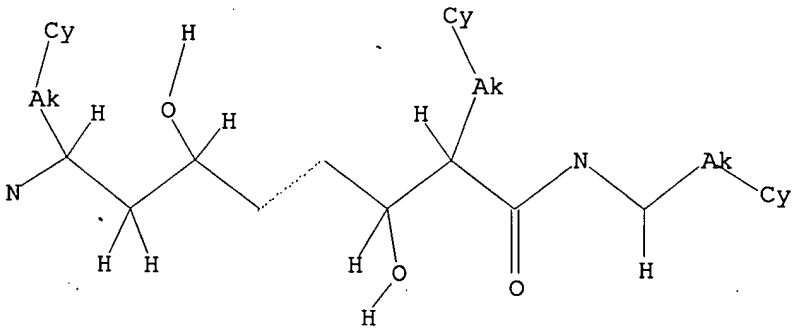
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10683756-2.str

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l5 full
FULL SEARCH INITIATED 15:02:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 147523 TO ITERATE

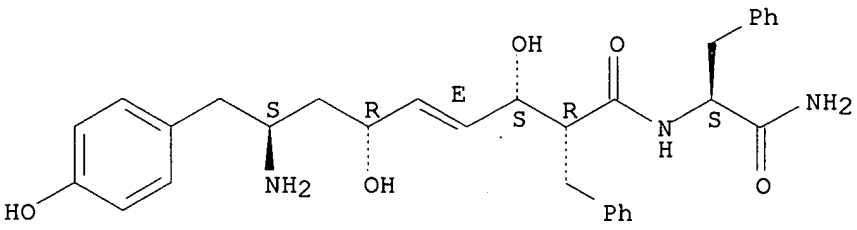
100.0% PROCESSED 147523 ITERATIONS 16 ANSWERS
SEARCH TIME: 00.00.09

L6 16 SEA SSS FUL L5

=> d 16 scan

L6 16 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenepropanamide, α-[(1S,2E,4R,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI)
MF C31 H37 N3 O5

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.38	351.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

FILE 'CAPLUS' ENTERED AT 15:03:28 ON 10 NOV 2006
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FILE COVERS 1907 - 10 Nov 2006 VOL 145 ISS 21
FILE LAST UPDATED: 9 Nov 2006 (20061109/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

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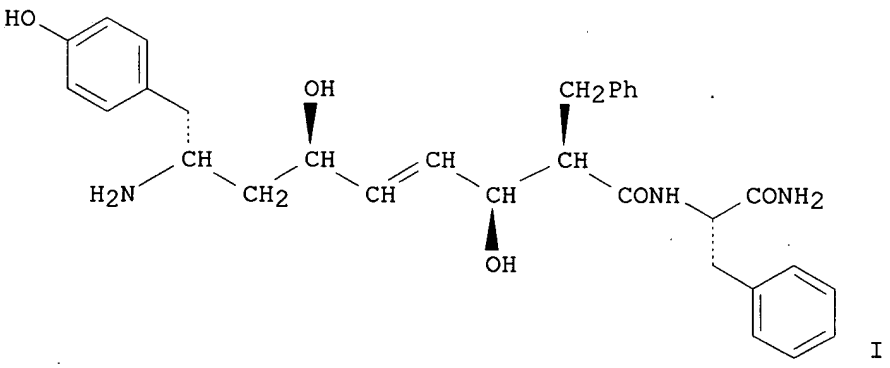
=> s l6 not l4
2 L6
L7 1 L6 NOT L4

=> d l7 abs ibib hitstr 1-
YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I

AB Using olefin cross-metathesis, the authors synthesized a novel stereodiversified library of I containing a trans-1,4-enediol. Screening this library for mu opioid receptor (MOR) affinity identified multiple high-affinity ligands and revealed that the stereochem. configuration varied widely among those ligands having the highest affinity. It was not possible to predict the configurations of the most active I stereoisomers on the basis of the configuration of endomorphin-2, a known MOR peptide ligand, validating the diversity-based approach to ligand discovery.

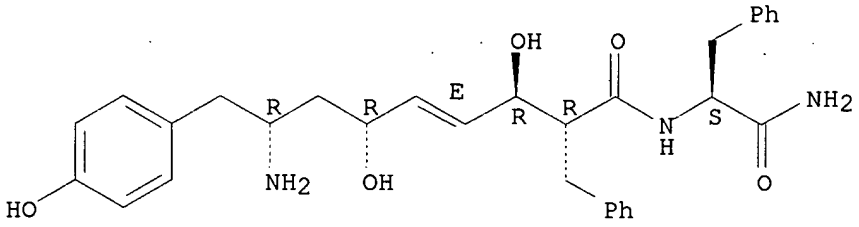
ACCESSION NUMBER: 2003:110339 CAPLUS
DOCUMENT NUMBER: 138:297095
TITLE: Unpredictable Stereochemical Preferences for Mu Opioid Receptor Activity in an Exhaustively Stereodiversified Library of 1,4-Enediols
AUTHOR(S): Shi, Zhangjie; Harrison, Bryce A.; Verdine, Gregory L.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Organic Letters (2003), 5(5), 633-636
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:297095
IT 507276-41-7P 507276-43-9P 507276-45-1P
507276-47-3P 507276-49-5P 507276-51-9P
507276-53-1P 507276-55-3P 507276-57-5P
507276-59-7P 507276-61-1P 507276-63-3P
507276-65-5P 507276-67-7P 507276-69-9P
507276-71-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(unpredictable stereochem. preferences for mu opioid receptor activity in an exhaustively stereodiversified library of enediols in relation to partial agonist activity)

RN 507276-41-7 CAPLUS

CN Benzenepropanamide, α-[(1R,2E,4R,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

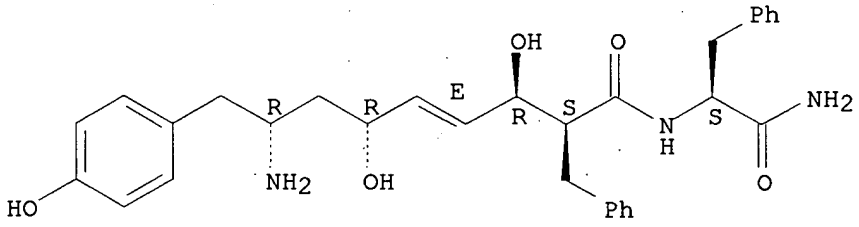
Absolute stereochemistry.
Double bond geometry as shown.



RN 507276-43-9 CAPLUS

CN Benzenepropanamide, α-[(1R,2E,4R,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

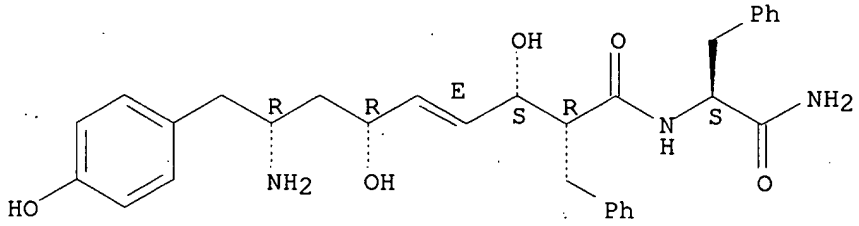
Absolute stereochemistry.
Double bond geometry as shown.



RN 507276-45-1 CAPLUS

CN Benzenepropanamide, α-[(1S,2E,4R,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

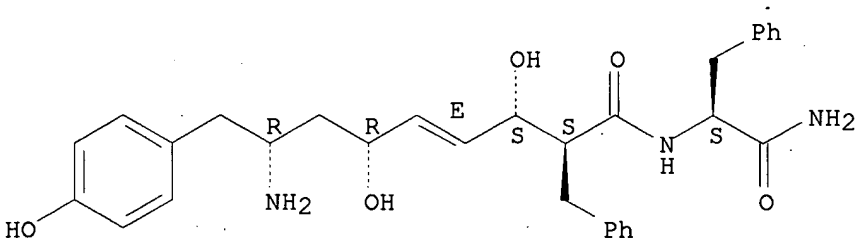
Absolute stereochemistry.
Double bond geometry as shown.



RN 507276-47-3 CAPLUS

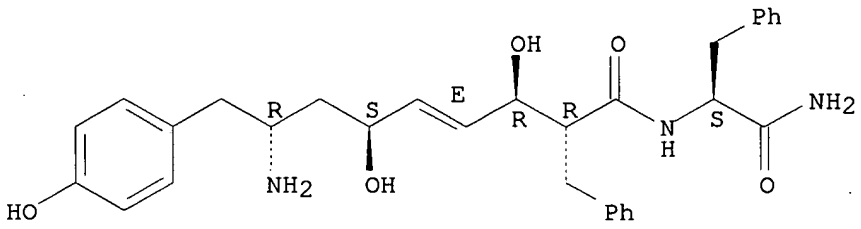
CN Benzenepropanamide, α-[(1S,2E,4R,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



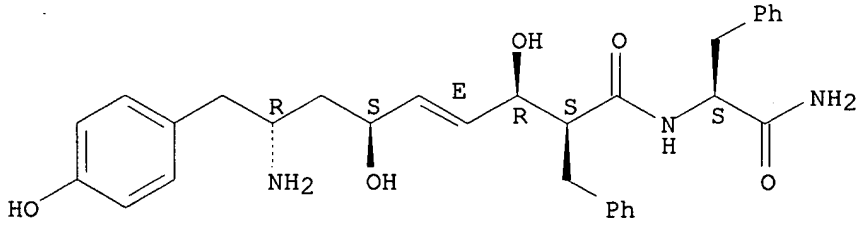
RN 507276-49-5 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,4S,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



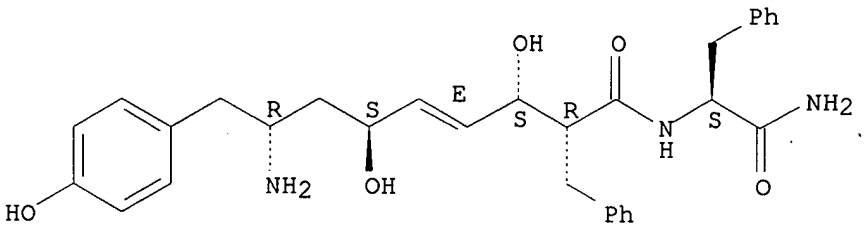
RN 507276-51-9 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,4S,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



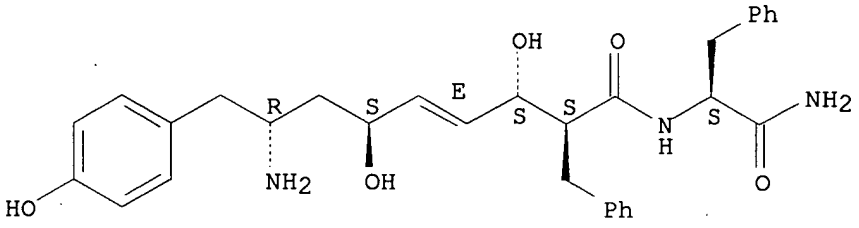
RN 507276-53-1 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,4S,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



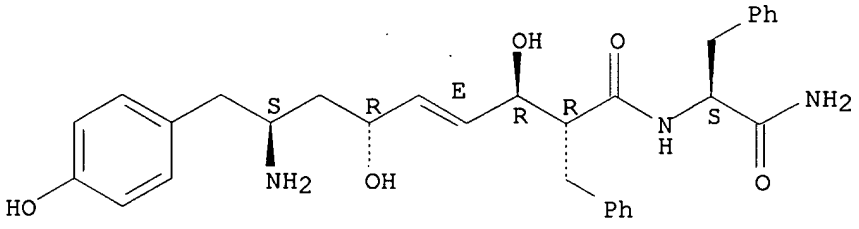
RN 507276-55-3 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,4S,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



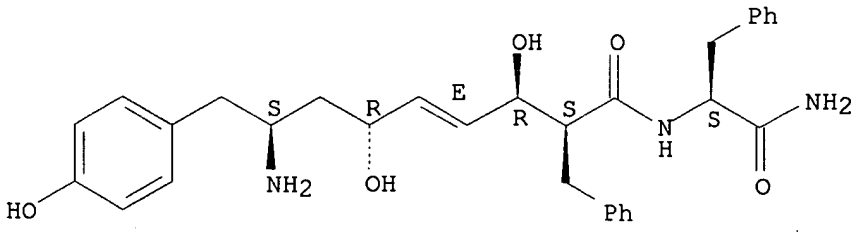
RN 507276-57-5 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,4R,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



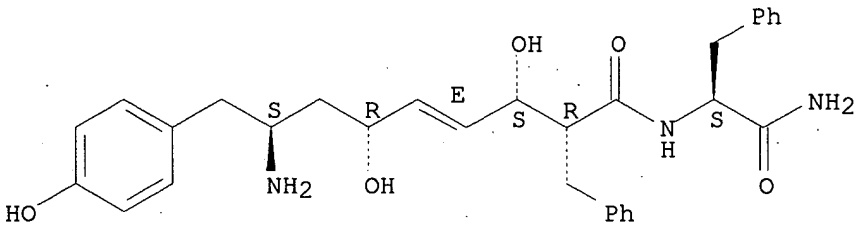
RN 507276-59-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,4R,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



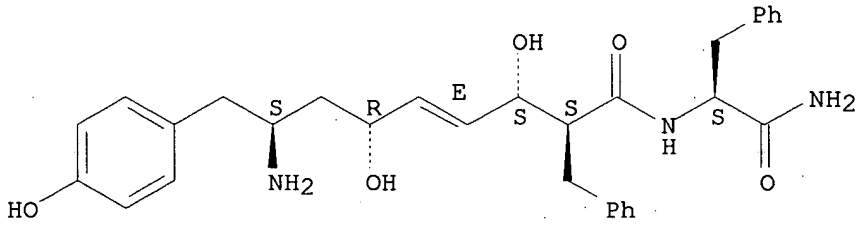
RN 507276-61-1 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,4R,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



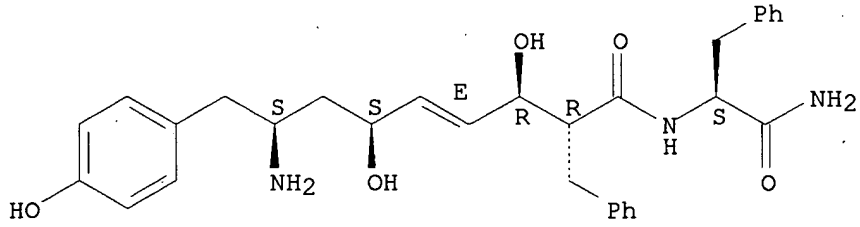
RN 507276-63-3 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,4R,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



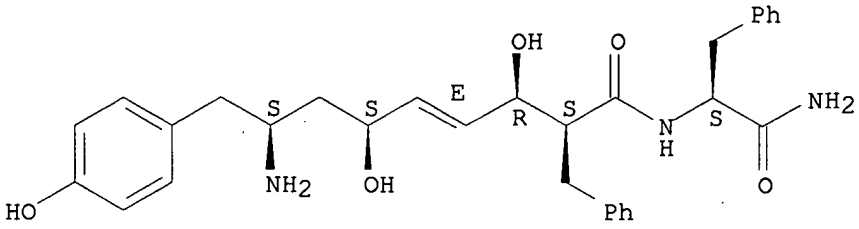
RN 507276-65-5 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,4S,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



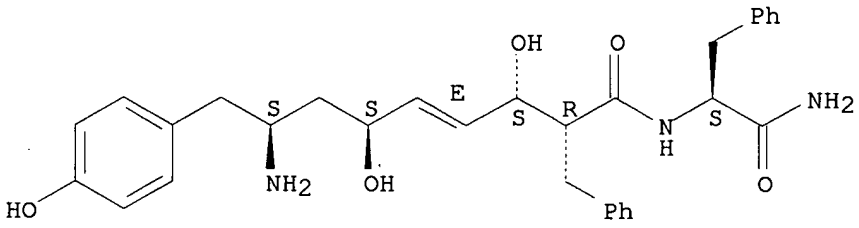
RN 507276-67-7 CAPLUS
CN Benzenepropanamide, α-[(1R,2E,4S,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 507276-69-9 CAPLUS
CN Benzenepropanamide, α-[(1S,2E,4S,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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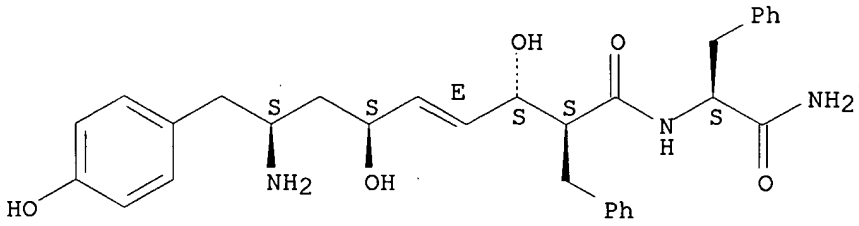
CN Benzenepropanamide, α-[(1S,2E,4S,6S)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT